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TABLE 15-continued

M <sub>6</sub> C. Err. d = 3%, err. $\phi$ = 1 deg. Elements: Fe, Nb.					
CODE	Formula	d <sub>1</sub> (largest)	d <sub>2</sub>	$\phi$	0
H727408	B18Fe76Nb6	6.25	3.82	90.0	

TABLE 16

ZrH <sub>2</sub> , data from Reference 13. d <sub>1</sub> = 4.912, d <sub>2</sub> = 3.367, $\phi$ = 90.0. Err. d = 2%, err. $\phi$ = 1.0 deg. Element: Zr.					
CODE	Formula	d <sub>1</sub> (largest)	d <sub>2</sub>	$\phi$	027550
102483	ZrH2	4.993.32	90.0		

TABLE 17

Search Simulations. CS = crystal system: A = anorthic(triclinic), M = monoclinic, O = orthorhombic, T = tetragonal, R = rhombohedral, H = hexagonal, C = cubic. First Entry for each phase is maximum d <sub>1</sub> , d <sub>2</sub> . Second entry is minimum d <sub>1</sub> , d <sub>2</sub> . Error limits: 1.5%, 1 deg.								
CODE	Name	Formula	CS	d1	d2	phi	Hits/Corr.	Hits/Corr. Red. Cell
000449	Albite	Na(Si3Al)O8	A	6.38	6.38	86.4	12/11	6/6
				4.02	3.78	70.6	13/13	
038274	Aragonite	CaCO3	O	7.96	5.73	90.0	7/6	6/6
				3.75	3.39	82.4	6/6	
038065	Calcite	CaCO3	R	5.68	4.19	75.8	9/9	7/7
				2.68	2.49	90.0	10/7	
003505	Gypsum	CaSO4·2H2O	M	7.58	5.37	69.3	7/7	7/7
				3.55	3.17	86.0	7/7	
033122	Halite	NaCl	C	3.25	3.25	70.5	3/3	3/3
				1.99	1.70	90.0	4/3	
001144	Kaolinite	Al2(OH)4Si2O5	A	8.95	7.14	88.1	2/2	1/2
				4.12	3.68	72.4	6/6	
003676	Molybdate	MoO3	O	13.9	3.96	90.0	5/5	4/4
				2.70	2.65	86.0	5/5	
024148	Pyrite	FeS2	C	5.41	5.41	90.0	12/10	12/12
				3.83	3.12	90.0	12/10	
026970	Quartz	SiO2	H	5.40	4.25	90.0	24/23	22/22
				3.34	2.28	71.8	29/29	
807069	Zircon	ZrSiO4	T	4.66	4.66	90.0	17/14	14/14
				2.98	2.64	63.7	14/14	

It will be apparent from the foregoing that many other variations and modifications may be made regarding the methods described herein, without departing substantially from the essential features and concepts of the present invention. Accordingly, it should be clearly understood that the forms of the invention described herein are exemplary only and are not intended as limitations on the scope of the present invention as defined in the appended claims.

What is claimed is:

1. A method for creating a searchable database of crystal electron diffraction data comprising:

- (a) creating tables within a relational database, said tables comprising Code data, Formula data, and Element data; wherein said Code data includes information relating to the d-spacings and acute angles of diffraction patterns of crystals, said Formula data includes information relating to the chemical formulae of said crystals, and said Element data includes information relating to the presence of elements of high atomic number in said crystals;

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(b) creating at least one macro for performing searches using said tables; said at least one macro including the steps of:

- (i) requesting input data relating to observed d-spacings, acute angles, experimental error limits, and anticipated atomic numbers of an experimental sample;
- (ii) comparing said input data with the data in said tables in accordance with said experimental error limits; and
- (iii) generating at least one report listing the crystals within said tables that match said input data.

2. The method for creating a searchable database of crystal electron diffraction data according to claim 1, wherein said Code data is derived from reduced unit cell parameters, and said step of comparing said input data includes calculating d-spacings produced by double diffraction.

3. A method for classifying crystal electron diffraction data obtained from an experimental sample, comprising:

(a) generating a relational database comprising:

- (i) at least three tables holding Code data, Formula data, and Element data, respectively; wherein said Code data includes information relating to the d-spacings and acute angles of diffraction patterns of crystals, said Formula data includes information relating to the chemical formulae of said crystals, and said Element data includes information relating to the presence of elements of high atomic number in said crystals;
- (ii) at least one macro for performing searches using said tables; said at least one macro including the steps of:
  - (1) requesting input data relating to observed d-spacings, acute angles, experimental error limits, and anticipated atomic numbers of an experimental sample;
  - (2) comparing said input data with the data in said tables in accordance with said experimental error limits; and